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THE KINETICS OF NEON-LIKE SELENIUM

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Abstract

In the recent successful demonstration of a soft x-ray laser in neon-like selenium, the 3p-3s J = 0 - 1 transition, which had been predicted to show very high gain, did not appear to be amplified. Most previous calculations have assumed that the dominant pumping mechanism is electron collisional excitation, and have neglected the effects of ionization and recombination on the kinetics of neon-like levels. In this work, we studied the effects of collisional ionization and three-body, radiative, and dielectronic recombination, connecting the three fluorine-like ground states to the lowest 89 levels of neon-like Se. Our results show that dielectronic recombination is a significant process for populating the J = 2 upper laser levels, and must be considered to model accurately the excited state kinetics of the neon-like ion.

The recent successful demonstration of a soft x-ray laser in neon-like selenium[1] raised a number of interesting puzzles. Perhaps the most intriguing is the fact that the $2p^5 3p$ - $2p^5 3s$ ($J = 0 - 1$) transition near 183 Å, which was predicted to have very high gain in all previous calculations,[2-4] did not show significant amplification.

The mechanism for creating the population inversion has been assumed to be collisional excitation from the neon-like ground state. For this reason, several predictions[2,3] have been based on kinetic models which included only neon-like states, and did not explicitly consider ionization or recombination from nearby ionization stages. Even calculations[4] which included other ionization stages treated dielectronic recombination in a simple way and neglected its effect on the populations of excited levels.

In this paper, we consider the effects of ionization and recombination, including detailed dielectronic recombination rates, which couple the fluorine-like ground states and the neon-like levels. We show that dielectronic recombination is an important mechanism for populating the $n = 3$ excited states of the neon-like ion and that it has significant effects on the $2p^5 3p$ - $2p^5 3s$ inversion kinetics. However, it is not in itself enough to explain the apparent lack of amplification of the $J = 0 - 1$ transition observed in the experiments.[1]

We constructed a kinetic model for selenium which included the $2s^2 2p^6$ ($J = 0$) neon-like ground state, the 36 $n = 3$ and the 52 $n = 4$ excited states, and the three fluorine-like states $2s^2 2p^5$ (J = 1/2, 3/2) and $2s2p^6$ (J = 1/2). Energies and radiative rates were computed using configuration interaction wave functions in intermediate coupling. For the n = 2 and n = 3 states of Ne-like selenium, we used the atomic structure code SUPERSTRUCTURE,[5] for the n = 4 states of Ne-like ion and the F-like states, the multiconfigurational Dirac-Fock code YODA.[6]

All collisional excitation rates were calculated by averaging collision strengths over a Maxwellian electron distribution. For the n = 2-3 transitions, the distorted wave code DSW[7] was used to compute L-S scattering amplitudes, which were transformed to intermediate coupling using JAJOM.[8] The n = 2-4 collision strengths were calculated directly in intermediate coupling using the relativistic distorted wave code MCDW.[6] The electron collision strengths for the electric dipole allowed, excited state-excited state transitions in the Ne-like ion, and the 2s-2p transitions in the F-like ion, were calculated using the classical path method.[9] Finally, the collision strengths for transitions among the fine-structure levels of a given n = 3 configuration [e.g., $(2p^5 3p)\ J \rightarrow 2p^5 3p\ J'$] were computed with DSW and JAJOM.

Ionization and three-body recombination rates were calculated using the scaled hydrogenic rates of Sampson and coworkers.[10] Radiative recombination rates were obtained using the prescription of Weisheit, et al.[11] All these rates are given by simple formulae which do not take into account the detailed structure of the states.

For the plasma conditions relevant for the neon-like selenium laser,[4] the dominant recombination process is dielectronic recombination, which we treated in full detail for all the ($3\ell 3\ell'$) and ($3\ell 4\ell'$) doubly excited states of Ne-like selenium. The dielectronic recombination coefficients were calculated in the isolated resonance approximation.[12] The Auger and radiative rates of the individual doubly excited states were evaluated in intermediate coupling with configuration interaction using the multi-configuration Dirac-Fock method.[12,13]

To study the excited state kinetics, we constructed rate equations and solved them in steady state for the level populations. We then calculated the relative inversion density for a given transition as:

$$y_{UL} = \nu_U - g_U \, \nu_L / g_L,$$

where ν_U (ν_L) and g_U (g_L) are the relative population and statistical weight, respectively, of the upper (lower) state of the transition. (Relative population is defined as the fraction of neon-like ions in a particular excited state.) We then calculated the gain coefficient of a Doppler broadened line from the expression:

$$\alpha = \frac{\lambda^3 A}{8\pi} \left[\frac{M_i}{2\pi k T_i}\right]^{1/2} y_{UL} \, n_{Ne}$$

where λ and A are the wavelength and radiative decay rate, respectively, of the lasing transition, M_i and T_i are the mass and temperature, respectively, of the ion, and n_{Ne} is the total density of Ne-like ions. We have taken the plasma parameters for our calculations to be those characteristic of the neon-like selenium laser plasma:[4] $n_e = 5 \times 10^{20}$ cm^{-3}, T_e = 1000 eV, T_i = 400 eV, and $n_{Ne} = 5 \times 10^{18}$ cm^{-3}. We assumed that the fraction of Ne-like ions is 0.25.

The importance of dielectronic recombination in determining the kinetics of the Ne-like excited states, of course, depends on the relative numbers of F- and Ne-like ions present. Models which include the F-like ionization stage will predict a F-like/Ne-like ratio (n_F/n_{Ne}). In our case, this ratio cannot be expected to be entirely correct since we have made no attempt to accurately determine the ionization balance. However, it should be noted that we found a reasonable n_F/n_{Ne} ratio, i.e., our value agreed within a factor of two with that obtained from steady-state ionization balance calculations[14] for $1 \times 10^{20} < n_e < 8 \times 10^{21}$ cm^{-3}. We also varied n_F/n_{Ne} artificially between 0.1 and 3.0 by introducing a multiplier for the collisional ionization rates.

The relative effects of cascade and dielectronic recombination on the inversion kinetics is shown in Table 1, where we compare results for models with different processes included. (For this comparison the collisional ionization multiplier is taken to be one.) Column 1 shows results obtained with a model containing only the Ne-like ground state and the n = 3 excited states (Ne37). In this case all excited state population comes directly or indirectly from the

Ne-like ground state. Column 2 shows results for a model containing the n = 2, 3, and 4 Ne-like states (Ne89). A comparison of columns 1 and 2 shows that collisional and radiative cascades alone increase the gain coefficient of the J = 2 - 1 transitions by 15-20%. Column 3 shows the results for a model (Ne37/F3) which adds the three F-like ground states to the Ne37 model, as well as ionization and recombination between the two ion stages. In this case, dielectronic recombination rates are summed over the (3131') excited states only. By comparing columns 1 and 3, we see that, even for a relatively small value of n_F/n_{Ne}, dielectronic recombination alone increases the gain coefficient of the J = 2 - 1 transitions by about 20-25%, and slightly decreases the J = 0 - 1 gain. Finally, column 4 gives results for a model (Ne89/F3), which includes both dielectronic recombination through the (3131') and (3141') Ne-like doubly excited states, and cascades from the n = 4 Ne-like excited states. In this case, the gain coefficient of the J = 2 - 1 transitions increases by 35-40% relative to the Ne37 case. The J = 0 - 1 transition decreases by about 10%, mostly due to an increase in population for the $2p^5 3s$ lower level.

Figure 1 shows the effects of varying n_F/n_{Ne} on the gain coefficients of the three transitions. When the number of F-like ions is small, the J = 0 - 1 transition has about the same gain coefficient as the larger of the two J = 2 - 1 transitions. As n_F/n_{Ne} increases the gains of the J = 2 - 1 transitions increase, and that of the J = 0 - 1 decreases slightly. This is because dielectronic recombination favors states with high statistical weight. Thus, the J = 2 states receive substantial population directly from the F-like ground state. The recombination rate into the J = 0 state is smaller, and does not compete with the very large collisional excitation rate from the Ne-like ground state. The small drop in gain for the J = 0 - 1 transition occurs because the $2p^5 3s$ (J = 1) lower level is also being populated by dielectronic recombination. We see from this figure that n_F/n_{Ne} must be very large for the gain of the J = 0 - 1 transition to be significantly reduced.

Determining the actual ionization balance of the x-ray laser plasma is an extremely difficult problem because it is not in steady state, and there are temporal and spatial gradients in the plasma during the amplified spontaneous emission. We have no direct measurement of the ionization balance, and the prediction of different codes do not agree. Based on qualitative information provided by time-resolved, n=2-3, x-ray spectra recorded during the experiments,[1,4] we believe that n_F/n_{Ne} is between 0.5 and 2.0.

Finally, Table 2 shows the results of varying the electron temperature in the calculation. We see that the relative inversion densities of the J = 2 - 1 transitions rise substantially compared to that of the J = 0 - 1 transition as the temperature rises. This is due primarily to the fact that the proportion of F-like ions rises rapidly with temperature.

These simple calculations cannot be expected to produce quantitative predictions for the gain coefficients. However, they clearly demonstrate that a model containing only the n = 2 and n = 3 states of Ne-like selenium is inadequate to calculate accurate level populations for the Ne-like excited states. The $2p^5 3p$ ($J = 0$) state is populated almost entirely by the rapid collisional excitation from the Ne-like ground state, and its population is not significantly affected by cascade from higher levels or by dielectronic recombination. However, the $2p^5 3p$ ($J = 2$) upper laser states (and, to a lesser extent, the $2p^5 3s$ ($J = 1$) lower states) are populated by collisional cascade from more highly excited states of the Ne-like ion (e.g., the $2s^2 2p^5 3d$, $2s2p^6 3p$ and $2s^2 2p^5 4l$ states) and by dielectronic recombination from the F-like ground states, as well as by direct collisional excitation from the Ne-like ground state. As a result, the gain coefficients of the transitions involving these states are sensitive to the ionization balance, i. e., n_F/n_{Ne}.

We have also found that including the ($3l4l'$) neon-like doubly excited states significantly increases the total dielectronic recombination rate. The contribution from the higher autoionizing states (e.g., $3\ell n\ell'$ with $n > 5$ and $n\ell n'\ell'$ with $n, n'>4$), neglected in the present calculations, are estimated to be 30-40% based on the results for Na-like Se.[15] The contribution from $\Delta n=o$ (Coster-Kronig) transitions peaks at much lower temperature (T_e = 60 eV) and is only 2% of the total rate at T_e = 1 keV.

Finally, it is clear that dielectronic recombination alone does not explain the experimental result[1] that the $J = 0 - 1$ transition did not exhibit significant amplification. The inversion density of this transition is reduced only slightly by this mechanism for reasonable values of n_F/n_{Ne}. In order to explain the absence of this line, a mechanism is required which either reduces the population of the $2p^5 3p$ ($J = 0$) upper state or absorbs the emitted photons.

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FIGURE CAPTION

FIG. 1. Gain coefficient (in cm^{-1}) of the three relevant $2p^5 3p$ - $2p^5 3s$ transitions in Ne-like selenium as a function of n_F/n_{Ne}.
1) J = 0 - 1 transition at 183 Å, 2) J = 2 - 1 transition at 209 Å, 3) J = 2 - 1 transition at 206 Å.

Table I. Effects of n = 4-3 cascades and dielectronic recombination on gain coefficients (cm^{-1}) of some $2p^5 3p$ - $2p^5 3s$ transitions in neon-like selenium.

Transition	Wavelength (Å)		Model			
			Ne37	Ne89	Ne37/F3	Ne89/F3
		n_F/n_{Ne}:	0.0	0.0	0.8	0.6
J = 0 - 1	183		14.3	13.4	13.9	13.0
J = 2 - 1	209		11.4	13.0	13.8	15.3
J = 2 - 1	206		9.7	11.5	12.1	13.6

Table II. Effect of electron temperature on the relative inversion density ($10^{-3}cm^{-3}$) for some $2p^53p$ - $2p^53s$ transitions of neon-like selenium.

T_e(eV)	Transition J = 0 - 1 (183Å)	J = 2 - 1 (209 Å)	J = 2 - 1 (206 Å)
500	.65	.71	1.4
1000	2.5	3.1	5.7
2000	4.2	6.4	11.

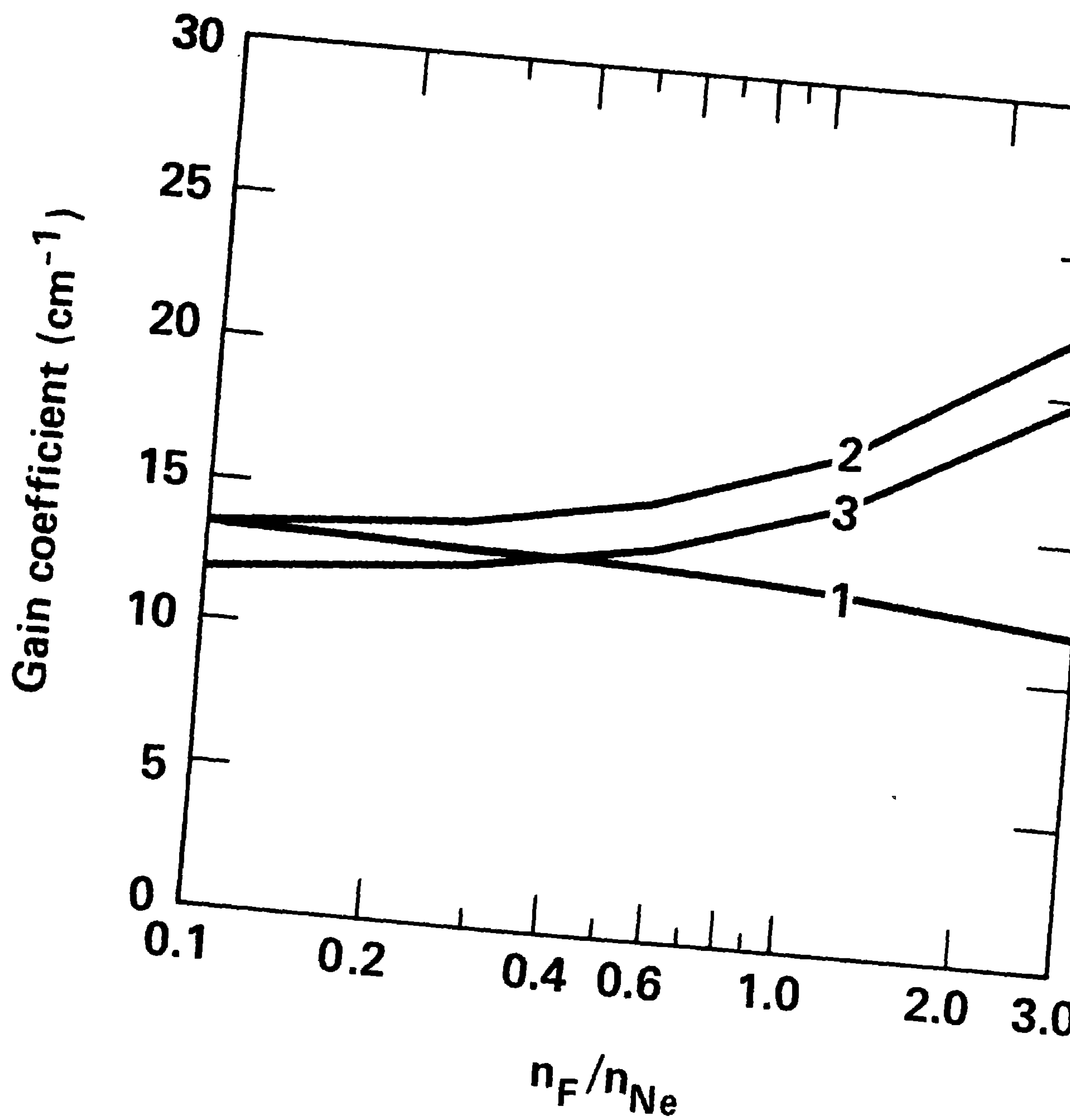
Gain coefficient (cm^{-1})
30
25
20
15
10
5
0
0.1
0.2
0.4
0.6
1.0
2.0
3.0
n_F/n_{Ne}
1
2
3

Figure 1